94. **PROCESS COST MODEL (WBS NO. 1512)**
$250,000
DOE Contact: Robert B. Schulz, (202) 586-8051
ORNL Contact: S. G. Winslow, (423) 574-0965
AlliedSignal Ceramic Components Contact:
B. S. Draskovich, (312) 512-5654

The objective of this new effort is to refine and utilize a process cost model for the evaluation of various fabrication methods used to manufacture diesel engine and aerospace/industrial turbomachinery structural ceramic components and provide a report containing an analysis of the process cost modeling effort.

Keywords: Cost-Effective Ceramics, Cost Reduction, Modeling, Processing, Structural Ceramics

OFFICE OF PROPULSION SYSTEMS

The Office of Propulsion Systems is comprised of the Advanced Propulsion Division and the Electric and Hybrid Propulsion Division. R&D programs focus on developing the technologies that will lead to the production and introduction of advanced heat engine propulsion systems, and electric and hybrid vehicles, in the Nation's transportation fleet. Technology development is conducted in concert with industry through cost-shared contracts. Materials activities of the Office of Propulsion Systems focus on integration of materials into components, and testing of subsystems for advanced vehicle propulsion systems.

ADVANCED PROPULSION DIVISION

The Advanced Propulsion Division consists of two programs: (1) Light Duty Engine Technologies Program, targeting Turbine Engine Technologies and Advanced Piston Engine Technologies; and (2) Heavy Duty Engine Technologies Program, targeting Advanced Diesel Engine Technology. Materials activities are supported by the Advanced Propulsion Division and managed through the NASA Lewis Research Center and the Oak Ridge National Laboratory. The DOE Contacts are: Thomas Sebestyen, (202) 586-8012 for Turbine Engine Technologies; Patrick Sutton, (202) 586-8058 for Automotive Piston Engine Technologies; and John Fairbanks, (202) 586-8066 for Heavy Duty Engine Technologies.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

95. **NASA SUPPORTING RESEARCH AND TECHNOLOGY**
$100,000
DOE Contact: Thomas Sebestyen, (202) 586-8012
NASA Contact: Thomas Strom, (216) 433-3408

The objective of this program is to evaluate commercially available structural and glass ceramic material specimens exposed to combustion products at temperatures up to 2500°F for periods up to 3,500 hours. Activities include: development of design codes for structural component evaluation; research on non-destructive evaluation of ceramic components to improve reliability; and examination of the effects of corrosive sea salts and other adverse environments on the durability of ceramics.

Keywords: Structural Ceramics, Nondestructive Evaluation, Silicon Carbide, Silicon Nitride, Gas Turbine Engines

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

96. **HYBRID VEHICLE TURBINE ENGINE (HVTE) TECHNOLOGY SUPPORT**
$3,600,000
DOE Contact: Thomas Sebestyen, (202) 586-8012
NASA Contact: Paul Kerwin, (216) 433-3409
Allison Engine Company Contact: Steve Berenyi, (317) 230-6971

The Hybrid Vehicle Turbine Engine (HVTE) Technology Support Program focuses on the DOE Hybrid Vehicle Program turbine engines in the 20-60kW size for hybrid vehicle application. In support of the advanced HVTE, Allison is designing, fabricating, and testing low-emission combustors, ceramic hot section components, a high performance ceramic regenerator core and seal system and cost-effective high temperature insulation system. Test rigs and test bed engines are being used to evaluate full-scale component and subsystem reliability and durability at cyclic operating conditions that are typical of automotive use at up to 2500°F.

Keywords: Structural Ceramics, Component Design, Silicon Carbide, Silicon Nitride, Gas Turbine Engines, Rig and Engine Testing

97. **CERAMIC TURBINE (CT) ENGINE DEMONSTRATION PROJECT**
$3,500,000
DOE Contact: Thomas Sebestyen, (202) 586-8012
NASA Contact: Thomas Strom, (216) 433-3408
AlliedSignal Engine Contact: Jay Smyth, (602) 231-4306

In support of the DOE Hybrid Vehicle Program, this project will provide early ceramic turbine field experience by demonstrating the reliability and durability of ceramic components in actual engine application. To this end, AlliedSignal began introducing ceramic first stage turbine nozzles and blades into its proven, available (all-metal) GTCP 331-200 gas turbine Auxilliary Power Unit (APU) engine. Laboratory and field testing is continuing to address remaining critical design and production concerns related to structural ceramics in gas turbine engines. In addition, efforts are intensified to scale-up and demonstrate commercial engine ceramic component manufacturing in coordination with ceramic suppliers and the Propulsion System Materials element of DOE's Materials Technology Program.

Keywords: Structural Ceramics, Component Design, Fabrication, Gas Turbine Engines, Component Testing

98. **ADVANCED DIESEL ENGINE COMPONENT DEVELOPMENT PROJECT**
$100,000
DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Mark J. Valco, (216) 433-3717
Detroit Diesel Corporation Contact: Jim Hoelzer, (313) 592-5565

The objective of the project is to develop advanced technology diesel engine components and integrate them into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative, and tribological component applications.

Keywords: Structural Ceramics, Low Heat Rejection Diesel Engines, Thermal Barrier Coatings, Component Designs, Composite Materials

99. **ADVANCED PISTON AND CYLINDER COMPONENT DEVELOPMENT**
$70,000
DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Mark J. Valco, (216) 433-3717
Caterpillar Inc. Contact: G. L. Waltz, (309) 578-6549

The objective of the project is to develop advanced technology diesel engine components and integrate them into a test bed engine to demonstrate reduced emissions and improved fuel economy. Advanced ceramic and metallic materials are being investigated and used in structural, insulative, and tribological component applications. Zirconia coatings are being used on piston crowns and composite pistons are being tested.

Keywords: Structural Ceramics, Low Heat Rejection Diesel Engines, Thermal Barrier Coatings, Component Designs, Composite Materials

100. **ADVANCED PISTON AND CYLINDER COMPONENT DEVELOPMENT**
$150,000
DOE Contact: John W. Fairbanks, (202) 586-8066
NASA Contact: Mark J. Valco, (216) 433-3717
Cummins Engine Contact: T. Yonushonis, (812) 377-7078

The objective of the project is to develop advanced technology diesel engine components and integrate these into a test bed engine to demonstrate reduced emissions and improved fuel economy. Nickel aluminides and Titanium aluminides are being investigated for turbocharger turbine rotors. Cast-in-place titanium nitride exhaust and intake port liners are emerging with improved reliability. Several powder metallurgy parts are being tested and zirconia and mullite coatings are being developed for piston crowns.

Keywords: Structural Ceramics, Low Heat Rejection Diesel Engines, Thermal Barrier Coatings, Component Designs, Composite Materials

101. **MICROWAVE REGENERATED PARTICULATE TRAP**
$75,000
DOE Contact: John W. Fairbanks, (202) 586-8066
ORNL Contact: Ronald Graves, (423) 574-2036

The objective of this project is to develop a particulate trap with fiber-reinforced (SiC) materials which will permit regeneration by heating with microwave energy. This will be done by utilizing a chemical vapor infiltration process to partially densify a thin fibrous substrate and produce a porous filter with high microwave coupling. This project is

being performed in collaboration with Cummins, Fleetguard, ReMaxCo and Microwave Materials Technology.

Keywords: Particulate Traps, Microwave Regeneration, Chemical Vapor Infiltration, Silicon Carbide Fibers, Low Heat Rejection Diesel Engines

ELECTRIC AND HYBRID PROPULSION DIVISION

The Electric and Hybrid Propulsion Division has three major programs: Battery Development, Fuel Cell Development, and Systems Development for electric vehicles. The DOE Contact is Kenneth Heitner, (202) 586-2341 for Battery Development; Steve Chalk, (202) 586-3388 for Fuel Cell Development; and Albert Landgrebe, (202) 586-1483 for Exploratory Research in support of Batteries and Fuel Cells.

MATERIALS PREPARATION, SYNTHESIS, DEPOSITION, GROWTH OR FORMING

102. **ELECTROCHEMICAL PROPERTIES OF SOLID-STATE SODIUM/POLYMER CELLS**
$275,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact:
L. C. De Jonghe, (510) 486-4881

The objective of this project is to investigate the viability of all-solid-state cells based on Na or Na alloy negative electrodes, polymeric electrolytes, and metal oxide positive electrodes. Emphasis is placed on developing a suitable cathode material not only in terms of performance but also in terms of cost and environmental impact. The approach is to synthesize and characterize manganese oxides for use as a cathode in Na/polymer cells and employ AC and DC techniques (e.g., galvanostatic charging and discharging, four probe techniques, and pulse testing) to characterize solid state batteries, as well as the properties of the individual components and interfaces. A full set of transport property measurements for the PEO/Na triflate system was completed. Especially noteworthy was the development of a new method of measuring transference numbers using straightforward electrochemical techniques, and a rigorous theoretical treatment of the results.

Keywords: Batteries, Solid-State Cells, Electric Vehicles, Polymeric Electrolytes

103. **IMPROVED CONTAINER ELECTRODE COATINGS FOR SODIUM/SULFUR BATTERY SYSTEMS**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Environmental Research Institute of Michigan
Contact: T. K. Hunt, (313) 667-2113

The objective of this project was to develop improved corrosion-resistant coatings for high-temperature secondary batteries by sputter-deposition techniques. Research was aimed at determining the utility of titanium films as durable, corrosion protective, conductive coatings for the sulfur electrodes in Na/S batteries. Several series of sputter-deposited TiN coatings were applied to Al coupons and the resulting samples soaked in Na_2S_4 at temperatures up to 390°C for 500 hours. The sputtering conditions were modified during the test series and the latter coatings showed no visible signs of corrosion following the 500 hour exposure. This project has been completed.

Keywords: Coatings, Na/S Batteries, Sputter-Deposition

104. **THE PERFORMANCE OF NEW MATERIALS FOR POLYMER ELECTROLYTE BATTERIES**
$140,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Northwestern University Contact: D. F. Shriver, (708) 491-5655

The objective of this project is to synthesize polymer electrolytes based on aluminosilicate-polyether hybrid polyelectrolyte with improved low-temperature performance and high cation transport number. These polymer electrolytes should be useful in rechargeable Li/polymer batteries. Initial efforts have focused on cell testing with simple polymer-salt electrolytes. This includes cycling with a cathode consisting of 70 percent Li_xMnO_2, 15 percent carbon, 15 percent polymer electrolyte, and a Li-metal anode. High cell capacity (135 mAh/g active cathode material) can be achieved at low discharge current. Experiments are underway to investigate the cause of the capacity fade that occurs with cycling. The data from these cells will provide a baseline for comparison with more advanced polyelectrolytes such as aluminosilicate-polyether hybrid polyelectrolyte.

Keywords: Polymer Electrolytes, Electrochemical Cells

105. **NOVEL POLYMER ELECTROLYTES FOR RECHARGEABLE LITHIUM BATTERIES**
$180,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Case Western University Contact: M. Litt, (216) 368-4174

The objective of this research is to develop advanced polymeric electrolytes for rechargeable Li batteries. Thin polymeric films are cast and characterized by spectroscopic, nuclear magnetic resonance, thermal and electrochemical techniques. Two types of polymer materials are under investigation: sulfonated and phosphonated polybenzimidazole polymers, and novel poly (4,5-dimethyleneimidazole and hydroxy imidazole) polymers. Currently, efforts are focused on preparing the polymer electrolytes and measuring their conductivities.

Keywords: Polymeric Electrolytes, Li Batteries

106. **NOVEL SOLID POLYMER ELECTROLYTES FOR ADVANCED SECONDARY BATTERIES**
$110,000
DOE Contact: JoAnn Milliken, (202) 586-2480
University of Dayton Contact: D. G. Glasgow, (513) 229-2517

The objective of this research program is to synthesize and characterize new polymer electrolytes that contain crown ethers which could improve the Li-ion transport. The systems proposed are doped polymers with side chains having the ability to form liquid crystalline (LC) mesophases. A novel LC monomer has been prepared and photopolymerized together with a monomer/salt mixture. Studies to align the polymer in an electric field are underway. Future efforts will focus on completing synthesis of polymer electrolytes and characterization of the polymers with respect to ionic conductivity, dimensional stability, and interfacial stability.

Keywords: Polymeric Electrolytes, Li Batteries, Ion Transport

107. **SOL-GEL ELECTROLYTES IN LITHIUM BATTERIES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Rutgers University Contact: L. C. Klein, (908) 932-2096

The objective of this research project was to optimize the synthesis of polymer electrolytes by sol-gel processing of alkali/silicate components, which involves combining the components in liquid form prior to chemically reacting the solution with water to form a gel. These materials should produce solid electrolyte compositions that can be applied directly to electrode materials for rechargeable Li batteries. The approach used in this investigation was to select oxide components that are Li-ion conductors and are thermodynamically stable. Alumina-containing formulations were identified which showed improved thermodynamic stability. This project has been completed.

Keywords: Sol Gel Electrolytes, Li Batteries, Polymer Electrolytes

108. **NEW CATHODE MATERIALS**
$155,000
DOE Contact: JoAnn Milliken, (202) 586-2480
State University of New York Contact: M. S. Whittingham, (607) 777-4623

The objective of this project is to synthesize and evaluate oxides of tungsten, molybdenum, and first-row transition metals for alkali-metal intercalation electrodes which are useful as positive electrodes in advanced nonaqueous rechargeable batteries. Mild hydrothermal techniques are used for the synthesis of molybdenum oxides, or, in cases where the hydrothermal technique does not lead to compounds with the highest oxidation state, electrochemical oxidation from an aqueous alkaline solution is used to drive the cations to their highest oxidation state. Hexagonal Mo oxides were prepared which have a greater capacity for Li intercalation than the normal MoO_3 phase. Layered structures were produced which should allow for rapid diffusion of Li ions. This research will be expanded to synthesize and test vanadium and manganese oxides.

Keywords: Intercalation Electrodes, Rechargeable Batteries

109. **DEVELOPMENT OF HIGH ENERGY DENSITY CATHODES FOR SODIUM/POLYMER CELLS**
$165,000
DOE Contact: JoAnn Milliken, (202) 586-2480
SRI International Contact: S. Smedley, (415) 859-6173

The major objective of this research is to develop high-performance organic polydisulfide positive electrodes for use in low-temperature (ambient to 100°C) Na/polymer cells. This will be achieved by the synthesis and characterization of hexathiobenzene-based compounds and their derivatives for positive electrodes. Specific parameters under investigation include the nature of any heteroatoms or side chains added to the base polymer, the structure of the polymer, the cathode thickness, the voltage stability window of the cathode, the degree of loading of the positive electrode material, the electrode construction technique, and the operating temperature of the cell. A cathode utilization of 164 mAh/g was achieved

for poly (hexathiobenzene), with an energy density of 260 Wh/kg at the C/10 rate at 95°C. Optimization of the cathode formulation should significantly improve cathode behavior.

Keywords: Cathodes, Na/polymer Cells, Electrochemical Analysis

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

110. **SURFACE MORPHOLOGY OF METALS IN ELECTRO-DEPOSITION/CARBON ELECTROCHEMISTRY**
$270,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contacts: K. Kinoshita and C. Tobias, (510) 486-4260

The objective of this project is to develop a pragmatic understanding of the component processes and their interactions in the macrocrystallization of metals necessary for the design and optimization of rechargeable galvanic cells. This project involves investigation of: (1) the role of electric field and solution-side mass transport in the electrocrystallization of metals, mechanisms of initiation, growth and propagation of imperfections, and development of surface textures; (2) the characterization of gases at electrodes with emphasis on their effect on ohmic resistance and mass transfer; and (3) the role of physicochemical properties of carbonaceous materials on their ability to reversibly intercalate Li. Results have shown that the initial velocity of the interface joining two bubbles depends on the bubble size and surface tension, but not on the electrolyte viscosity. In addition a mathematical model has been completed to understand the hydrodynamics of flow over protrusions. Analysis of existing data suggests that the mechanism and capacity for intercalation of Li may differ between the highly ordered graphites and less ordered carbons.

Keywords: Macrocrystallization of Metals, Galvanic Cells, Li Batteries

111. **FABRICATION & TESTING OF CARBON ELECTRODES AS LITHIUM INTERCALATION ANODES**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Livermore National Laboratory Contact: R. Pekala, (510) 422-0142

The objectives of this work are to evaluate the performance of carbonaceous materials as hosts for lithium intercalation negative electrodes, and to develop reversible lithium intercalation negative electrodes for advanced rechargeable lithium batteries. The approach is to fabricate electrodes from various commercial carbons and graphites and evaluate them in small lithium-ion cells. Electrode performance will be correlated with carbon structure and properties in collaboration with LBNL. Electrodes fabricated from various Lonza graphites yielded Li intercalation capacities that range from 320 to 365 mAh/g (equivalent to x in Li_xC_6 from 0.85 to 0.95), approaching the theoretical value of 372 mAh/g.

Keywords: Carbon, Li Batteries, Intercalation

112. **BATTERY MATERIALS: STRUCTURE AND CHARACTERIZATION**
$150,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4071

The objective of this research is to elucidate the molecular aspects of materials and electrode processes in batteries and to use this information to develop electrode and electrolyte structures with good performance and long life. Current efforts have included *in situ* extended x-ray absorption fine structure (EXAFS) studies of Bi-doped manganese oxides and *ex situ* studies of lithium manganese oxides and nickel oxide electrodes that were cycled in Zn/NiOOH cells. Results have shown that corrosion of Ni plaque is the failure mode for sintered nickel oxide electrodes. No chemical interaction was observed between zincate and nickel hydroxide. Decreases in nickel oxide capacity in zinc/nickel oxide cells are most likely due to pore plugging by ZnO. Future efforts will focus on EXAFS studies of additives in nickel oxide and zinc electrodes as well as studies of molybdenum and tungsten oxide electrodes.

Keywords: Electrodes, Batteries, EXAFS

113. ***IN SITU* SPECTROSCOPIC APPLICATIONS TO THE STUDY OF RECHARGEABLE LITHIUM BATTERIES**
$150,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Case Western Reserve University Contact: D. A. Scherson, (216) 368-5186

The purpose of this project is to use *in situ* spectroscopic techniques to investigate the electrochemical phenomena that occur at Li/electrolyte interfaces during charge/discharge cycling. The approach is to conduct experimental studies under ultrahigh vacuum conditions to examine the reactivity of Li at the Li/polymer and Li/liquid electrolyte interfaces. Attenuated Total Reflection-Fourier Transform Infrared (ATR-FTIR) Spectroscopy indicates that no reaction occurs at the Li/PEO interface. Modifications found in the ATR-FTIR spectrum following Li deposition

and stripping are most likely caused by changes in the polymer morphology.

Keywords: Spectrographic Analysis, Electrochemical Phenomena, Electrolytes

114. **POLYMER ELECTROLYTE FOR AMBIENT TEMPERATURE TRACTION BATTERIES: MOLECULAR LEVEL MODELING FOR CONDUCTIVITY OPTIMIZATION**
$160,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Northwestern University Contact: M. A. Ratner, (708) 491-5371

The goal of this research is to apply molecular dynamics (MD) and Monte Carlo simulations to understand the conduction process in polymer electrolytes, and its modification by such parameters as temperature, density, ion species, polymer chain basicity, and interionic correlations. The results of this study should be beneficial in the development of improved polymer electrolytes for rechargeable Li batteries for EV applications. MD simulations have shown that there are very few free ions in polymer/salt electrolytes of the stoichiometry usually measured. Hopping models have demonstrated that the conductivity is fixed by the segmental relaxation of the polymer host and by the number of free ions.

Keywords: Batteries, Electric Vehicles, Polymeric Electrolytes

115. **ANALYSIS AND SIMULATION OF ELECTROCHEMICAL SYSTEMS**
$240,000
DOE Contact: JoAnn Milliken, (202) 586-2480
University of California, Berkeley Contact: J. Newman, (510) 642-4063

The objective of this program is to improve the performance of electrochemical cells used in the interconversion of electrical energy and chemical energy by identifying the phenomena which control the performance of a system. These phenomena are incorporated into a mathematical model which can predict system behavior. The models aid in the recognition of important parameters that are crucial to the optimization of a given electrochemical system. Computer techniques with electrochemical engineering principles permit the calculation of complex interactions without gross mathematical and physical approximations. A model which describes the impedance response of a rechargeable Li battery at open circuit has been developed. The nickel/metal hydride battery has been modeled in both one-dimensional and full two-dimensional form. A model has also been developed which predicts the behavior of electrochemical double layer capacitors under operating conditions.

Keywords: Electrochemical Phenomena, Galvanostatic Charge/Discharge

116. **HEAT TRANSPORT AND THERMAL MANAGEMENT IN ADVANCED BATTERIES**
$175,000
DOE Contact: JoAnn Milliken, (202) 586-2480
University of California, Berkeley Contact: J. W. Evans, (510) 642-3807

This project was initiated in FY 1995 to investigate, by mathematical modeling and experimental measurement, heat generation and transport in advanced secondary batteries for electric vehicle (EV) applications. The objectives of this project are to evaluate the management of the temperature of the battery for optimum performance and to avoid temperature excursions damaging to the battery. Initial investigations were focused on Li/polymer batteries that are under development to operate in the temperature range of approximately 60 to 140°C, which is required to obtain sufficient polymer conductivity and to avoid overheating. A two-dimensional mathematical model revealed that the major resistance to heat transport in a Li/polymer-electrolyte battery is the polymer electrolyte.

Keywords: Thermal Modeling, Advanced Batteries

117. **ELECTRODE SURFACE LAYERS**
$140,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: F. R. McLarnon, (510) 486-4260

Advanced *in situ* and *ex situ* characterization techniques are being used to study the structure, composition, and mode of formation of surface layers on electrodes used in rechargeable batteries. The objective of this research is to identify film properties that improve the rechargeability, cycle-life performance, specific power, specific energy, stability, and energy efficiency of electrochemical cells. Sensitive techniques such as ellipsometry, light scattering, Raman spectroscopy and scanning electron microscopy are utilized to monitor the formation of surface layers on secondary battery electrodes. In addition, foreign ions are incorporated in porous nickel electrodes to improve the cycle performance in an alkaline electrolyte. A newly developed technique for low-energy ion implantation was used to implant Au, Pb, Ta, Ti, W, and Ti_4O_7 in nickel oxide electrodes. Tests showed that the overpotential for oxygen evolution at the surface of a Ti_4O_7-implanted Ni

electrode is increased by 50-105 mV, compared with electrodes implanted with other elements.

Keywords: Ion Implantation, Electrodes, Rechargeable Batteries

118. **ELECTRODE KINETICS AND ELECTROCATLYSIS**
$400,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: P. N. Ross and E. J. Cairns, (510) 486-6226

Physically meaningful mechanistic models are essential for the interpretation of electrode behavior and are useful in directing the research on new classes of materials for electrochemical energy conversion and storage devices. The objective of this project is to develop an atomic-level understanding of the processes taking place in complex electrochemical reactions at electrode surfaces. Researchers are employing low energy electron diffraction (LEED) to study single crystals; high resolution electron microscopy (HREM) for carbon electrode materials; and X-ray absoption fine structure (EXAFS) for organometallic catalysts. Low Energy Ion Scattering (LEIS) and Auger Electron Spectroscopy (AES) are being utilized to study the composition of sputtered and UHV-annealed polycrystalline Pt-Ru bulk alloys for methanol electrocatalysis. It was found that the property of Ru atoms to nucleate oxygen-containing species at low potentials produced a strong enhancement in the catalytic activity of sputter-cleaned Pt-Ru alloy electrodes compared to pure Pt, thereby supporting the concept of the bifunctional character of the oxidation process of these alloys.

Keywords: Spectrographic Analysis, Electrocatalysts, Electrooxidation

119. **EFFECT OF ELECTROCATALYST AND ELECTROLYTE COMPOSITION ON METHANOL/AIR FUEL CELL PERFORMANCE**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: E. J. Cairns and P. N. Ross, (510) 486-6226

There is a strong need to develop a fuel cell that can electrochemically oxidize liquid fuels, and the successful development of a direct-methanol fuel cell (DMFC) would represent a major advance for fuel-cell-powered vehicles. However, some major obstacles such as oxidation rate must be addressed before acceptable performance can be attained. The objective of this project is to elucidate the mechanism of methanol electrooxidation on electrocatalysts for DMFCs. Results have shown that the optimum surface composition of Pt-Ru varied with temperature and the shift in optimum composition with temperature can be attributed to a shift in the rate-determining step from CH_3OH adsorption/dehydrogenation at room temperature to the surface reaction between the dehydrogenated intermediate and surface oxygen at 60°C. Fuel cells with 20-cm^2 electrodes were designed and fabricated. Studies of the direct electrochemical oxidation of methanol and hydrocarbon fuels in liquid alkali carbonate and Solid Polymer Electrolytes (SPEs), respectively, are underway.

Keywords: Electrooxidation, Fuel Cells

120. **POISONING OF FUEL CELL ELECTROCATALYST SURFACES: NMR SPECTROSCOPIC STUDIES**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: E. J. Cairns, (510) 486-5028

Platinum is the most active single-component catalyst for CH_3OH electrooxidation in DMFCs; however, poisoning reactions at the surface render the anode ineffective under target operation conditions. The objective of this research is to obtain information on the nature of the poisoning intermediate(s) in CH_3OH electrooxidation on Pt-based electrocatalysts by NMR. Experiments are currently underway to determine the feasibility of NMR to detect surface poisons during methanol electrooxidation.

Keywords: NMR, Electrooxidation, Fuel Cells

121. **FUEL CELLS FOR RENEWABLE APPLICATIONS**
$1,000,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Los Alamos National Laboratory Contact: S. Gottesfeld, (505) 667-0853

The primary focus of this program is to develop efficient and cost-effective polymer electrolyte fuel cells (PEFC) for transportation applications. The specific goals of the program are to: (1) reduce the cost of the Pt catalyst and ionomeric membrane, (2) increase the efficiency and power density of the PEFC, (3) optimize the system for operation on reformed organic fuels and air, (4) achieve stable, efficient, long-term operation, and (5) solve key technical issues that impede the development of the DMFC. For the first time, limiting currents significantly in excess of 2 A/cm^2 were obtained for hydrogen/air PEM fuel cells under ordinary operating conditions. Efforts will

continue to focus on improving the performance and life of PEM and DM fuel cells and identifying new low-cost components for these fuel cells.

Keywords: Fuel Cells, Proton Exchange Membranes, Methanol Oxidation

122. **ELECTROCATALYSIS OF FUEL CELL REACTIONS**
$100,000
DOE Contact: JoAnn Milliken, (202) 586-2480
Brookhaven National Laboratory Contact: J. McBreen, (516) 282-4513

The purpose of this project is to increase the understanding of electrocatalysis on a molecular level and to apply this knowledge to improve the performance of fuel cells for transportation applications. The goals are to reduce the Pt requirements for solid PEFCs, to develop non-Pt catalysts for oxygen reduction, and to identify catalysts for the direct oxidation of methanol. The approach is to use X-ray absorption (XAS) to study the chemical/electrochemical properties of fuel cell electrocatalysts. XAS results have shown that the electrocatalysis of small organic molecules on Pb-modified Pt cannot be attributed to adsorption of oxygen species on Pb, but rather depend on the disordered nature of the Pb adlayer. This project has been completed.

Keywords: Fuel Cells, Electrocatalysts, X-Ray Absorption

DEVICE OR COMPONENT FABRICATION, BEHAVIOR OR TESTING

123. **Zn/NiOOH CELL STUDIES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Berkeley Laboratory Contact: E. Cairns and F. McLarnon, (510) 486-4260

The purpose of this project was to investigate the behavior of Zn electrodes in alkaline Zn/NiOOH cells to improve their lifetime and performance. Zn/NiOOH batteries would provide superior performance and lower life-cycle costs compared to Cd/NiOOH and MH/NiOOH batteries. The approach of this project was to determine the performance and cycle life of alkaline Zn/NiOOH cells using realistic cell components and operating conditions as well as utilize analytical instruments such as X-ray diffraction analysis and XAS to understand changes to cell components resulting from charge/discharge cycling. X-ray photoelectron spectroscopy results have shown that the NiOOH electrode in the Zn/KOH/NiOOH cells do not chemically react with the Zn species under cycling conditions with a KOH-KF-K_2CO_3 electrolyte. A CRADA has been established with Energy Research Corporation to further technology transfer.

Keywords: Electrodes, Batteries, Electric Vehicles

124. **APPLIED RESEARCH ON SECONDARY Zn/NiOOH BATTERY TECHNOLOGY**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Acme Electric Corporation Contact: M. Anderman, (602) 921-0470

The objectives of this project were to evaluate the Lawrence Berkeley Laboratory (LBL) electrolyte composition for extending the cycle life of Zn/NiOOH cells, and to develop these cells for EV applications. Cells containing the LBL electrolyte were fabricated and results have shown that 175 charge/discharge cycles were completed. A visual examination of the electrodes showed a drastic improvement (reduction) in electrode shape change compared to the electrodes cycled in the standard, highly-alkaline electrolyte. This project has been completed.

Keywords: Electrodes, Batteries, Electric Vehicles

125. **DEVELOPMENT OF A THIN-FILM RECHARGEABLE LITHIUM BATTERY FOR ELECTRIC VEHICLES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Oak Ridge National Laboratory Contact: J. B. Bates, (615) 574-4143

The objective of this research is to identify methods for depositing acceptable thin-film electrodes for rechargeable Li batteries. These methods are being applied to develop solid-state $Li/Li_xMn_2O_4$ rechargeable thin-film Li batteries for EV applications. The batteries are expected to have several important advantages as power sources: high specific energy and energy density, long cycle lifetimes, and a wide temperature range of operation. Accomplishments have included fabrication of $Li/Li_x/Mn_2O_4$ cells in which the cathode was deposited at temperatures below 150°C by rf magnetron sputtering and fabrication of thin-film cells capable of sustaining current densities of several mA/cm^2, having a specific power of 30 W/g at an 85 C discharge rate. Cells exhibited less than 0.05 percent capacity loss per cycle after hundreds of cycles when discharged to 2-3 volts (~C/1). Efforts will focus on improving the performance of $Li_xMn_2O_4$ cathode films deposited at low temperatures and investigate the performance of a hybrid solid-state $Li\text{-}Li_xMn_2O_4$ cell.

Keywords: Electric Vehicles, Thin-Film Batteries, Solid-State Electrodes

126. **NA/SRPE ELECTRIC VEHICLE BATTERIES**
$200,000
DOE Contact: JoAnn Milliken, (202) 586-2480
PolyPlus Battery Company Contact: May-Ying Chu, (510) 841-4313

The purpose of this project is to demonstrate the cycling capability of cells containing Na negative and organosulfur-based positive electrodes, and develop a low-cost high-performance Na/polymer cell that utilizes an organosulfur-based positive electrode. The proposed batteries will be mechanically sturdy, have a reliable electrical performance, operate between 50 and 80°C, and are expected to be immune to thermal cycling. To date, approximately 80 laboratory Na/Solid Redox Polymer Electrolyte (SRPE) cells have been constructed and testing has been initiated. Maximum single discharge of 450 Wh/kg of cathode vs. Na and peak power of 800 W/kg of cathode vs. Na have been demonstrated. Limited cycling of 5 cycles above 250 Wh/kg and 20 cycles above 100 Wh/kg was achieved.

Keywords: Electrodes, Batteries, Electric Vehicles

127. **LITHIUM-ION BATTERY TESTING**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Lawrence Livermore National Laboratory Contact: S. Mayer, (510) 423-4897

The objective of this project was to evaluate the performance of Li-ion cells to determine their cycle life and energy/power characteristics under controlled conditions. In this study, cells manufactured by the Sony Corporation for use in portable electronic devices were tested. The capacity and specific energy of cells that were charged to 4.2 V were about 1 Ah and >94 Wh/kg, respectively. Cycle life exceeded 300 cycles under Dynamic Stress Test at 100 percent Depth of Discharge (DOD), and 2800 cycles at 44 percent DOD. This project has been completed.

Keywords: Li Batteries, Dynamic Stress Testing

128. **NOVEL CONCEPTS FOR AN OXYGEN ELECTRODE IN SECONDARY METAL-AIR BATTERIES**
$0
DOE Contact: JoAnn Milliken, (202) 586-2480
Eltech Research Corporation Contact: E. J. Rudd, (216) 357-4073

The objective of this research was to develop improved bifunctional air electrodes for electrically rechargeable Zn/air cells. The successful development of bifunctional air electrodes depends on selecting electrochemically stable support materials and electrocatalysts for O_2 reduction and evolution, and the fabrication of suitable porous structures that are capable of extended operation. In this program, the properties of corrosion-resistant substrates such as semi-graphitic carbon, graphite or non-carbon materials were investigated. Results show that electrodes with a graphitized acetylene black for the support and $NiCo_2O_4$ and either CoTMPP or $La_{0.6}Ca_{0.4}CoO_3$ as electrocatalysts have operated for over 100 cycles in 35 percent KOH at room temperature. This project has been completed.

Keywords: Metal-Air Batteries, Bifunctional Air Electrodes, Zn/Air Cells